

A discrete Hubbard-Stratonovich decomposition for general, fermionic two-body interactions

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Abstract

A scheme is presented to decompose the exponential of a two-body operator in a discrete sum over exponentials of one-body operators. This discrete decomposition can be used instead of the Hubbard-Stratonovich transformation in auxiliary-field quantum Monte-Carlo methods. As an illustration, the decomposition is applied to the Hubbard model, where it is equivalent to the discrete Hubbard-Stratonovich transformation introduced by Hirsch, and to the nuclear pairing Hamiltonian.

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I. INTRODUCTION

In auxiliary-field quantum Monte-Carlo methods (AFQMC), such as the projector, grand-canonical [1] and shell-model quantum Monte-Carlo methods [2], the Boltzmann operator $e^{-\beta\hat{h}}$, with \hat{h} the Hamiltonian, is decomposed in a sum or integral of exponentials of one-body operators. This sum or integral is then evaluated using Monte-Carlo techniques. For the decomposition, these methods rely on the Hubbard-Stratonovich transformation [3,4], which is based on the identity

$$e^{\beta\hat{\rho}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2}} e^{\sigma\sqrt{2\beta}\hat{\rho}} d\sigma, \quad (1)$$

where $\hat{\rho}$ is a one-body operator. In order to avoid problems due to non-commuting operators, one can split up the Boltzmann operator using the Suzuki-Trotter formula [5]. One can discretize the Hubbard-Stratonovich transformation by applying a Gaussian quadrature formula to the integral over σ . After a Suzuki-Trotter expansion in N_t slices, a three-points quadrature formula leads to an error of the order of $\mathcal{O}\left(\frac{\beta^3}{N_t^2}\hat{h}^3\right)$. This is of the same order in β and N_t as the errors due to the non-commutativity of the squared operators that build up \hat{h} . For some systems one can derive an exact, discrete Hubbard-Stratonovich transform. Hirsch showed how one can write an operator of the form $e^{-\beta U \hat{n}_\uparrow \hat{n}_\downarrow}$, where \hat{n}_σ is the site occupation number for an electron with spin projection σ , exactly as a sum of two exponentials of one-body operators [6]. Recently, Gunnarsson and Koch extended this to systems with higher orbital degeneracy [7].

The aim of this paper is to describe another discrete decomposition scheme, which is exact for a certain class of operators. This decomposition scheme is generalized to any two-body Hamiltonian using the Suzuki-Trotter formula. For the application in AFQMC methods, especially the shell-model Quantum Monte-Carlo method, this new decomposition has the advantage, compared to the discretized Hubbard-Stratonovich transform based on Eq.(1), that it is more accurate and that it leads to low-rank matrices. This leads to faster matrix multiplications and requires less computer memory. AFQMC methods for fermions often have sign problems [1]. Fahy and Hamann [8] showed that these sign problems can be related to the diffusive behavior of states in the Hubbard-Stratonovich transformation. Because our decomposition, in general, is based on exponentials of one-body operators of a completely different type, one can expect different sign properties. Our decomposition is not free of sign problems, but there might be systems where it leads to a sign rule while the Hubbard-Stratonovich transformation does not, or where our decomposition causes significantly less sign problems.

In Section II we introduce a matrix notation for Slater determinants and operators needed for a clear discussion of the decomposition. In Section III a basic lemma is given on which the decomposition is based. In Section IV the exact decomposition for a certain class of operators is presented. We indicate how to apply this decomposition to a general two-body Hamiltonian. In Section V the relation with Hirsch's decomposition for the Hubbard model is elucidated. Finally, in Section VI the decomposition for the nuclear pairing Hamiltonian is discussed and illustrated with AFQMC-results for an exactly solvable model.

II. A MATRIX NOTATION FOR SLATER DETERMINANTS AND OPERATORS

In order to avoid confusion between matrix representations in the space of single-particle states and the operators themselves in Fock space, we will denote the former with upper case and the latter with lower case characters. Let $\{\phi_1, \dots, \phi_{N_s}\}$ be a set of basis states for the single-particle space, $\hat{a}_1, \dots, \hat{a}_{N_s}$ be the related creation operators and the A -particle state Ψ_M the antisymmetrized product of a set of single-particle states $\sum_{i=1}^{N_s} M_{ij} \phi_i$, $j = 1 \dots A$. i.e. Ψ_M is a Slater determinant. Thus in second quantization one can write

$$|\Psi\rangle = \prod_{j=1}^A \left(\sum_{i=1}^{N_s} M_{ij} \hat{a}_i \right) |\rangle. \quad (2)$$

This defines a matrix representation M for a Slater determinant Ψ_M . The value of this representation is that one can represent certain operations on the Slater determinant by matrix operations on M . e.g. the overlap between two Slater determinants $\Psi_{M'}$ and Ψ_M is given by $\langle \Psi_M | \Psi_{M'} \rangle = \det(M^\dagger M')$. The exponential of a one-body operator acting on Ψ_M results in a new Slater determinant, $e^{-\beta \hat{h}} |\Psi_M\rangle = |\Psi_{M'}\rangle$ (this is a corollary of the Thouless-theorem [9]), whose matrix representation is related to M by $M' = e^{-\beta H} M$, where the $N_s \times N_s$ matrix H is defined by $\hat{h} = \sum_{i,j} H_{ij} \hat{a}_i^\dagger \hat{a}_j$. Reversily, given a $N_s \times N_s$ matrix Q , one can consider the operator $\hat{O}(Q)$, defined by its action on Slater determinants:

$$\hat{O}(Q) : |\Psi_M\rangle \longrightarrow \hat{O}(Q) |\Psi_M\rangle = |\Psi_{M'}\rangle \text{ with } M' = QM. \quad (3)$$

If Q is non-singular, $\hat{O}(Q)$ is the exponential of a one-body operator.

III. A BASIC LEMMA

Lemma: *The operation represented by the unit matrix plus a matrix of rank two can be expressed as a sum of one- and two-body operators in the following way:*

$$\hat{O}(1 + \alpha B_1^\dagger B_4 + \beta B_2^\dagger B_3) = 1 + \alpha \hat{b}_1^\dagger \hat{b}_4 + \beta \hat{b}_2^\dagger \hat{b}_3 + \alpha\beta \hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3 \hat{b}_4, \quad (4)$$

where B_1, B_2, B_3 and B_4 are $1 \times N_s$ row matrices and $\hat{b}_k = \sum_{j=1}^N (B_k)_j \hat{a}_j$, $k = 1, 2, 3, 4$.

Proof: Consider the A -particle Slater determinant Ψ_M represented by the matrix M . Consider also a Slater determinant Ψ_L , that has particles in the single-particle states $\phi_{i_1}, \phi_{i_2}, \dots, \phi_{i_A}$. The Slater determinants of this type constitute a basis of the A -particle Hilbert space. The overlap of Ψ_L with Ψ_M is given by

$$\langle \Psi_L | \Psi_M \rangle = \det(\tilde{M}_{.1} \tilde{M}_{.2} \dots \tilde{M}_{.A}). \quad (5)$$

The notation $M_{.j}$ denotes the vector that is given by the j^{th} column of M , the notation \tilde{B} for an N -element vector B denotes the A -element vector $(B_{i_1} B_{i_2} \dots B_{i_A})$. The operator in Eq.(4) transforms Ψ_M into $\Psi_{M'}$ with $M' = (1 + \alpha B_1^\dagger B_4 + \beta B_2^\dagger B_3)M$. To calculate the overlap of $\Psi_{M'}$ with Ψ_L , we have to replace every column $\tilde{M}_{.j}$ in Eq.(5):

$$\tilde{M}_{.j} \rightarrow \tilde{M}'_{.j} = \tilde{M}_{.j} + \alpha_j \tilde{B}_1^\dagger + \beta_j \tilde{B}_2^\dagger, \text{ with } \alpha_j = \alpha B_4 M_{.j}, \quad \beta_j = \beta B_3 M_{.j}. \quad (6)$$

The overlap is then given by

$$\langle \Psi_L | \Psi_{M'} \rangle = \det \left(\tilde{M}_{.1} + \alpha_1 \tilde{B}_1^\dagger + \beta_1 \tilde{B}_2^\dagger \quad \cdots \quad \tilde{M}_{.A} + \alpha_A \tilde{B}_1^\dagger + \beta_A \tilde{B}_2^\dagger \right). \quad (7)$$

This determinant can be expanded as the sum of all determinants that are obtained by selecting in every column of Eq.(7) one of the terms \tilde{M}_j , $\alpha_j \tilde{B}_1^\dagger$ or $\beta_j \tilde{B}_2^\dagger$. If in more than one column the term $\alpha_j \tilde{B}_1^\dagger$ is selected, then the determinant has two linearly dependent columns, so it will vanish. The same holds for the term $\beta_j \tilde{B}_2^\dagger$. Only four types of determinants remain:

- \tilde{M} is selected in every column. This determinant is just $\langle \Psi_L | \Psi_M \rangle$ (see Eq.(5)).
- $\alpha_j \tilde{B}_1^\dagger$ is selected in column j , \tilde{M} in all others. These determinants sum up to $\langle \Psi_L | \alpha \hat{b}_1^\dagger \hat{b}_4 | \Psi_M \rangle$ (one particle is moved from state b_4 to state b_1).
- $\beta_j \tilde{B}_2^\dagger$ is selected in column j , \tilde{M} in all others. These determinants sum up to $\langle \Psi_L | \beta \hat{b}_2^\dagger \hat{b}_3 | \Psi_M \rangle$ (one particle is moved from state b_3 to state b_2).
- $\alpha_j \tilde{B}_1^\dagger$ is selected in column j , $\beta_k \tilde{B}_2^\dagger$ is selected in column k , \tilde{M} in all others. These determinants sum up to $\langle \Psi_L | \alpha \beta \hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3 \hat{b}_4 | \Psi_M \rangle$ (two particles are moved from states b_4 and b_3 to states b_1 and b_2).

Taking all these terms together, we find that

$$\langle \Psi_L | \Psi_{M'} \rangle = \langle \Psi_L | 1 + \alpha \hat{b}_1^\dagger \hat{b}_4 + \beta \hat{b}_2^\dagger \hat{b}_3 + \alpha \beta \hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3 \hat{b}_4 | \Psi_M \rangle. \quad (8)$$

This holds for any basis state Ψ_L , so that

$$\Psi_{M'} = \left(1 + \alpha \hat{b}_1^\dagger \hat{b}_4 + \beta \hat{b}_2^\dagger \hat{b}_3 + \alpha \beta \hat{b}_1^\dagger \hat{b}_2^\dagger \hat{b}_3 \hat{b}_4 \right) \Psi_M. \quad (9)$$

This proves Eq.(4).

End of proof.

IV. A DISCRETE HUBABRD STRATONOVICH DECOMPOSITION

Consider a fermionic two-body operator \hat{Q} of the form

$$\hat{q} = \sum_{i,j,k,l=1}^{N_s} Q_{ij} (B_1)_k (B_2)_l \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k. \quad (10)$$

An operator of this form has the special property that

$$\hat{q}^2 = \lambda \hat{q}, \quad \text{with } \lambda = \sum_{k,l=1}^{N_s} (Q_{kl} - Q_{lk}) (B_1)_k (B_2)_l. \quad (11)$$

Because of this relation, the exponential of \hat{q} can be written as

$$e^{-\beta \hat{q}} = 1 + \gamma \hat{q}, \quad \text{with } \begin{cases} \gamma = \frac{e^{-\beta \lambda} - 1}{\lambda} & \text{for } \lambda \neq 0, \\ \gamma = -\beta & \text{if } \lambda = 0. \end{cases} \quad (12)$$

Now we can use the lemma to obtain a discrete decomposition of $e^{-\beta\hat{q}}$ in a sum of exponentials of one-body operators:

$$\begin{aligned} e^{-\beta\hat{q}} &= \sum_{i,j=1}^{N_s} \frac{1}{2} \sum_{\sigma=-1,+1} \frac{|Q_{ij}|}{\Theta} \left(1 + \sigma\chi_{ij}\hat{a}_i^\dagger\hat{b}_1 + \sigma\chi'_{ij}\hat{a}_j^\dagger\hat{b}_2 + \chi_{ij}\chi'_{ij}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{b}_2\hat{b}_1 \right), \\ &= \sum_{i,j=1}^{N_s} \sum_{\sigma=-1,+1} \frac{|Q_{ij}|}{2\Theta} \hat{\mathcal{O}} \left(1 + \sigma\chi_{ij}A_i^\dagger B_1 + \sigma\chi'_{ij}A_j^\dagger B_2 \right), \end{aligned} \quad (13)$$

with A_i the $1 \times N_s$ row matrix which has a 1 on the i^{th} entry and zeros anywhere else, and

$$\Theta = \sum_{i,j=1}^{N_s} |Q_{ij}|, \quad (14)$$

$$\chi_{ij} = \sqrt{|\gamma|\Theta}, \quad (15)$$

$$\chi'_{ij} = \sqrt{|\gamma|\Theta} \operatorname{sign}(\gamma Q_{ij}), \quad (16)$$

$$\hat{b}_k = \sum_{l=1}^{N_s} (B_k)_l \hat{a}_l, \quad k = 1, 2. \quad (17)$$

This is an exact Hubbard-Stratonovich-like decomposition of the form of Eq.(10). To apply this discrete Hubbard-Stratonovich-like decomposition to the Boltzmann operator $e^{-\beta\hat{v}}$ for a general fermionic two-body operator \hat{v} , one has to rewrite \hat{v} as a sum of operators of the form Eq.(10). A trivial way to do this, is given by

$$\hat{v} = \sum_{i,j,k,l=1}^{N_s} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k = \sum_{k,l=1}^{N_s} \hat{q}_{kl}, \quad \text{with } \hat{q}_{kl} = \left(\sum_{i,j=1}^{N_s} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \right) \hat{a}_l \hat{a}_k. \quad (18)$$

The Suzuki-Trotter formula can be used to split up the Boltzmann operator into factors with only one operator \hat{q}_{kl} in the exponent. Then each of these factors can be decomposed exactly using the discrete decomposition in Eq.(13). Note that the total decomposition is no longer exact because of the non-commutativity of the operators \hat{q}_{kl} . The error will be of the order $\mathcal{O}(\beta^3/N_t^2)$. It will be much smaller than in case of a decomposition based on a Gaussian discretization of the integral in Eq.(1), because now the error is proportional to the commutators of the operators \hat{q}_{kl} and no longer to a power of \hat{v} .

V. RELATION TO HIRSCH'S DECOMPOSITION FOR THE HUBBARD HAMILTONIAN

For the Hubbard model we have to find a decomposition for a Boltzmann operator of the form $e^{-\beta U \hat{n}_\uparrow \hat{n}_\downarrow}$, where U is the interaction strength and $\hat{n}_{i\sigma} = \hat{a}_\sigma^\dagger \hat{a}_\sigma$. $\sigma = \uparrow, \downarrow$ is an index for the spin degree-of-freedom. The exponent has a two-body operator $\hat{n}_\uparrow \hat{n}_\downarrow$, which is an operator of the form of Eq.(10), so we can apply the decomposition given in Eq.(13) and obtain:

$$e^{-\beta U \hat{n}_\uparrow \hat{n}_\downarrow} = \frac{1}{2} \sum_{\sigma=-1,+1} \hat{\mathcal{O}} (1 + \sigma\chi_\uparrow N_\uparrow + \sigma\chi_\downarrow N_\downarrow), \quad (19)$$

with $N_\uparrow(N_\downarrow)$ the matrix which is zero everywhere except for the diagonal element related to the spin-up (spin-down) site, which is equal to 1. χ and χ' are given by

$$\chi_\uparrow = -\chi_\downarrow = \sqrt{1 - e^{-\beta U}} \quad \text{for } \beta U > 0, \quad (20)$$

$$\text{or } \chi_\uparrow = \chi_\downarrow = \sqrt{e^{-\beta U} - 1} \quad \text{for } \beta U < 0. \quad (21)$$

Now one could scale each term in Eq.(19) with an operator of the form $e^{-\beta\mu(\hat{n}_\uparrow + \hat{n}_\downarrow)}$, because in the canonical ensemble this is just a constant. The matrices in the decomposition now have to be multiplied with the matrix $1 + (e^{-\beta\mu} - 1)N_\uparrow + (e^{-\beta\mu} - 1)N_\downarrow$. In case of the repulsive Hubbard model, the choice $\mu = -U/2$ leads to the discrete Hubbard-Stratonovich transform of Hirsch [6]. From the computational point of view this particular choice of μ has the advantage that the matrix representation for the spin-down part is related to the matrix representation for the spin-up part by a matrix inversion. Then one only has to keep track of the spin-up part in actual AFQMC calculations. Hirsch's decomposition for the attractive Hubbard model can also be obtained from Eq.(19), with a particular choice for μ . In this case however, there is no computational advantage in taking any particular value.

VI. APPLICATION TO THE NUCLEAR PAIRING HAMILTONIAN

The Hamiltonian for nuclear pairing in a degenerate shell is given by

$$\hat{h} = -G \sum_{k,k'=1}^{N_S} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}'} \hat{a}_{k'}. \quad (22)$$

Here it is assumed that there are $2N_S$ degenerate single-particle states. The single-particle energy is shifted to 0 MeV. So there is no one-body part in the Hamiltonian. The states with $j_z > 0$ are labeled from 1 to N_S and \bar{k} denotes the time-reversed state of state k . The many-body problem for this model can be solved analytically using the seniority scheme [10].

Using the Suzuki-Trotter formula, the Boltzmann operator for this Hamiltonian can be written as

$$e^{-\beta\hat{h}} = e^{-\frac{\beta}{2}\hat{q}_1} e^{-\frac{\beta}{2}\hat{q}_2} \dots e^{-\frac{\beta}{2}\hat{q}_{N_S}} e^{-\frac{\beta}{2}\hat{q}_{N_S}} \dots e^{-\frac{\beta}{2}\hat{q}_2} e^{-\frac{\beta}{2}\hat{q}_1} + \mathcal{O}(\beta^3), \quad (23)$$

with

$$\hat{q}_k = -G \left(\sum_{k'=1}^{N_S} \hat{a}_{k'}^\dagger \hat{a}_{\bar{k}'}^\dagger \right) \hat{a}_{\bar{k}} \hat{a}_k. \quad (24)$$

The error is of the order $\mathcal{O}(\beta^3)$. It is assumed that β is small. In practice, one has to split β in a number of inverse-temperature slices using the Suzuki-Trotter formula. Then one can apply the procedure that is discussed here to each inverse-temperature slice separately. We have $\hat{q}_k^2 = -G\hat{q}_k$. So we can find a decomposition of the type given in Eq.(13)

$$e^{-\frac{\beta}{2}\hat{q}_k} = \sum_{k'=1}^{N_S} \sum_{\sigma=-1,+1} \frac{1}{2N_S} \hat{\mathcal{O}} \left(1 + \sigma \chi A_{k'}^\dagger A_k + \sigma \chi A_{\bar{k}'}^\dagger A_{\bar{k}} \right), \quad (25)$$

where $\chi^2 = N_S \left(e^{\frac{\beta G}{2}} - 1 \right)$.

We have applied this decomposition to study a degenerate shell of 20 states ($N_S = 10$), with 10 particles. This could model the valence model space for neutrons in the fp shell in ^{56}Fe , if one neglects the energy gap between the $1f_{7/2}$ and the $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ orbitals. For the strength of the interaction we took $G = 20/\bar{A}$ MeV = 20/56 MeV, as recommended in [11]. We have performed a shell-model quantum Monte-Carlo calculation in the canonical ensemble, following [2], but now using the new decomposition of Eq.(25) instead of the Hubbard-Stratonovich transformation. In order to make the systematic error smaller than the statistical error, the inverse temperature β was split into slices of length 0.05 MeV^{-1} . We point out that the form $1 + \sigma \chi A_{k'}^\dagger A_k + \sigma \chi A_{\bar{k}'}^\dagger A_{\bar{k}}$ can be rewritten as $(1 + \sigma \chi A_{k'}^\dagger A_k) (1 + \sigma \chi A_{\bar{k}'}^\dagger A_{\bar{k}})$, such that there is a symmetry between states with $j_z > 0$ and their time-reversed states. This symmetry guarantees that there will be no sign problem for systems with an even number of particles. This sign-rule is analogous to the sign rule for the pairing-plus-quadrupole Hamiltonian decomposed using the Hubbard-Stratonovich transform [12]. In figure 1 we show the internal energy of the system as a function of temperature. In figure 2 we show the corresponding specific heat of the system as a function of temperature. The Monte-Carlo results are in excellent agreement with the analytical results. The peak in the specific-heat curve around a temperature of 0.8 MeV. can be associated with the breakup of $J^\pi = 0^+$ pairs. It is straightforward to take into account the different single-particles energies and more general forms of the pairing Hamiltonian:

$$\hat{h} = \sum_{k=1}^{N_S} \epsilon_k (\hat{n}_k + \hat{n}_{\bar{k}}) - \sum_{k,k'=1}^{N_S} G_{k,k'} \hat{a}_k^\dagger \hat{a}_{\bar{k}}^\dagger \hat{a}_{\bar{k}'} \hat{a}_{k'}. \quad (26)$$

Extension to even more general two-body Hamiltonians is possible. Then there can be sign problems at low temperatures.

VII. CONCLUSION

We have presented a new type of discrete Hubbard-Stratonovich decomposition for the Boltzmann operator. It is exact for a special class of two-body operators. Applied to the Hubbard Hamiltonian, it leads to Hisrch's discrete Hubbard-Stratonovich decomposition. The decomposition is well suited for the nuclear pairing Hamiltonian, where it leads to a sign rule for systems with an even number of particles. Quantum Monte-Carlo results based on this decomposition are in excellent agreement with the analytical results for an exactly solvable model.

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FIGURES

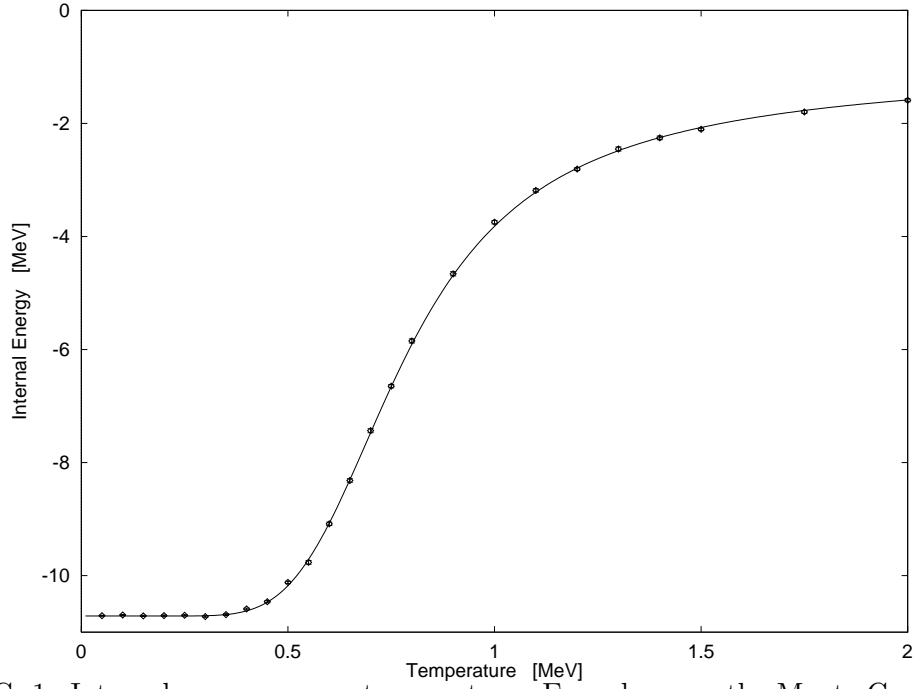


FIG. 1. Internal energy versus temperature. Error bars on the Monte-Carlo data are omitted because they are smaller than the symbols marking the data points.

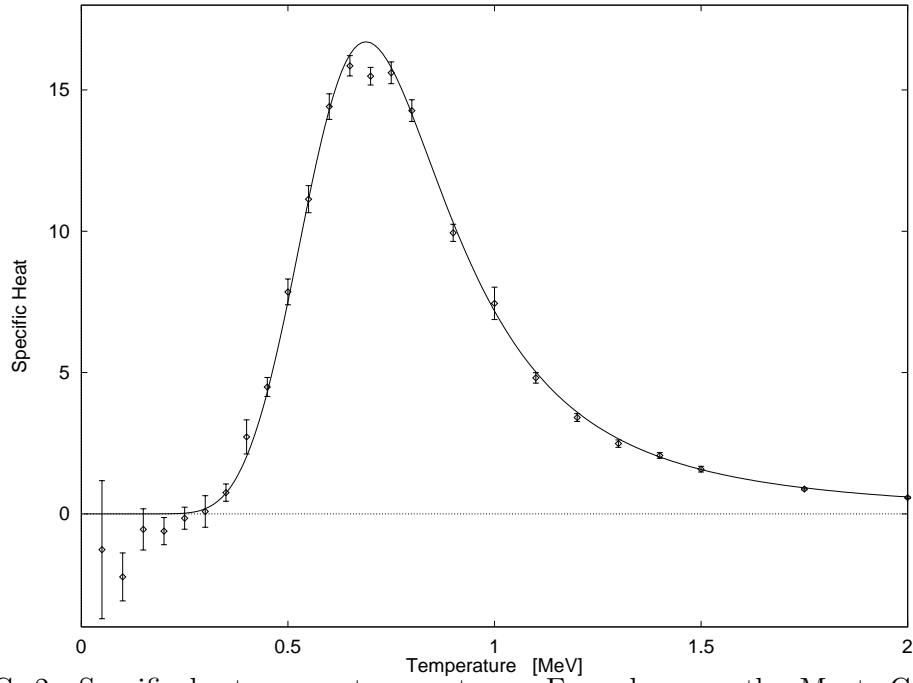


FIG. 2. Specific heat versus temperature. Error bars on the Monte-Carlo data represent 95%-confidence intervals.